

# Designing Langevin Microdynamics in Macrocosm

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Previously developed “stochastic representation of deterministic interactions” enables exact treatment of an open system without leaving its native phase space (Hilbert space) due to peculiar stochastic extension of Liouville (von Neumann) equation for its statistical operator. Can one reformulate the theory in terms of stochastic “Langevin equations” for its variables? Here it is shown that in case of classical Hamiltonian underlying dynamics the answer is principally positive, and general explicit method of constructing such equations is described.

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**I. Introduction.** Any Langevin equations involve irreversibility (friction) and indeterminism (noise), as the classical equations which imitate interaction between “Brownian particle” and a fluid (see e.g. [1] and references therein). Both the friction and noise represent the same reversible and deterministic microscopic dynamics, but usually are presumed unambiguously (additively) distinguishable. In general, of course, such assumption is wrong, because the friction itself can essentially fluctuate, as in the case of interaction between macroscopic vibrations of a quartz crystal and its own phonon gas (see e.g. [2] and references therein). Therefore the question arises: how one should construct “Langevin equations” (interpreted loosely as a model replacement of underlying microscopic dynamics) to be sure they result quite accurate and thus free of artifacts?

The answer can be formulated in the framework of “the stochastic representation of deterministic interactions” [4, 5, 6, 7, 8, 9], at least in two widespread situations:

i) when the dynamics is Hamiltonian while interaction between a system of interest, “D”, and other world, “B”, is described by a bilinear contribution to Hamiltonian of “D+B” [4, 5, 6, 9] :

$$H = H_d + H_b + H_{int} , \quad H_{int} = \sum_n D_n B_n ; \quad (1)$$

the marks “d” and “b” and the operators (or phase functions, in classical mechanics)  $D_n$  and  $B_n$  relate to “D” and “B”, respectively;

ii) when joint evolution operator of “D+B”,  $L$ , has similar bilinear form [6, 7] :

$$L = L_d + L_b + L_{int} , \quad L_{int} = \sum_n \Lambda_n^d \Lambda_n^b \quad (2)$$

The evolution operator is understood as those governing joint statistical operator,  $\rho$ , of “D+B”:

$$d\rho/dt = L\rho \quad (3)$$

In Hamiltonian dynamics,  $L = \mathcal{L}(H)$ , where  $\mathcal{L}(H)$  is quantum or classical Liouville operator,

$$\mathcal{L}(H)\rho = \frac{i}{\hbar}[\rho, H] \quad \text{or} \quad \mathcal{L}(H)\rho = \left( \frac{\partial H}{\partial q} \frac{\partial}{\partial p} - \frac{\partial H}{\partial p} \frac{\partial}{\partial q} \right) \rho ,$$

with  $\{q, p\}$  being canonic variables. In case (1)  $L = \mathcal{L}(H)$  always has the bilinear form (2) [6, 7] (the case (2) covers also non-canonic treatments of Hamiltonian dynamics [7] and, besides, essentially non-Hamiltonian and irreversible dynamics, and even Markovian probabilistic evolutions).

For simplicity, in this paper discussion of the Langevin equations will be confined by classical mechanics, moreover, starting from Sec.III, by the case (1) only.

**II. Characteristic functionals.** The statistical operator  $\rho$  from Eq.3 (density matrix, probability measure, etc.) says about current state  $\Gamma = \Gamma_d \oplus \Gamma_b$  of “D+B” only. Who is interested also in its correlations with its prehistory, may consider one or another characteristic functional (CF)

$$\begin{aligned} \text{Tr}_d \text{Tr}_b \rho(t, \Gamma) \left\langle \exp \left[ \int_{t>t'} \sum_j v_j(t') Q_j(\Gamma(t')) dt' \right] \right\rangle^\Gamma &\equiv \\ &\equiv \left\langle \exp \left[ \int_{t>t'} \sum_j v_j(t') Q_j(t') dt' \right] \right\rangle , \end{aligned} \quad (4)$$

where  $Q_j(\Gamma)$  are some phase functions (i.e. functions of instant system’s state) and  $v_j(t)$  conjugated arbitrary test functions (probe functions);  $\text{Tr}_b$  and  $\text{Tr}_d$  denote “traces” over phase spaces of “B” and “D”, that is integrations over  $\Gamma_b$  or  $\Gamma_d$ ;  $\langle \dots \rangle^\Gamma$  is conditional statistical average under given present state  $\Gamma = \Gamma(t)$ , and the right-hand side retells the left from viewpoint of exterior observers. Particularly, in case of deterministic dynamics the conditional averaging degenerates into replacing  $\Gamma(t')$  by strictly definite function of  $\Gamma = \Gamma(t)$ .

In any case, if readdressing symbol  $\rho$  to the whole expression under the traces in (4), one can write

$$\left\langle \exp \left[ \int_{t>t'} \sum_j v_j(t') Q_j(t') dt' \right] \right\rangle = \text{Tr}_d \text{Tr}_b \rho , \quad (5)$$

where now, obviously,  $\rho$  obeys the equation

$$d\rho/dt = \{ \sum_j v_j(t) Q_j(\Gamma) + L \} \rho \quad (6)$$

instead of (3). Thus one reduces CF to slightly modified evolution equation. In fact that is a sort of famous relations between path integrals and differential equations,

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like the Feynman-Kac formulas [10, 11]. Nevertheless, we once more accented the transition from (4) to (5)-(6) (see also Sec.2 in [8]) because, curiously, some referees are not familiar with such possibility (by the way, some similar old examples can be found in [12, 13]).

**III. Stochastic representation.** Consider partial probability measure of “D”’s states,  $\rho_d \equiv \text{Tr}_b \rho$ , where  $\rho$  satisfies the evolution equation (3). According to [4, 5, 6], if once  $\rho$  was factored, then later  $\rho_d$  can be represented as the average

$$\rho_d = \langle \langle \tilde{\rho}_d \rangle \rangle \quad (7)$$

of stochastic probability measure  $\tilde{\rho}_d$  which obeys the time-local differential equation

$$\frac{d\tilde{\rho}_d}{dt} = \left[ \sum_n y_n(t) D_n + \mathcal{L} \left( H_d + \sum_n x_n(t) D_n \right) \right] \tilde{\rho}_d \quad (8)$$

with  $x_n(t)$  and  $y_n(t)$  being definite stochastic processes and  $\langle \langle \dots \rangle \rangle \equiv \langle \langle \dots \rangle_y \rangle_x \equiv \langle \langle \dots \rangle_x \rangle_y$  statistical average with respect to them. Similarly, if the phase functions  $Q_j$  wholly belong to “D” then their CF (4) can be represented, in place of (5) and (6), as

$$\left\langle \exp \left[ \int_{t>t'} \sum_j v_j(t') Q_j(t') dt' \right] \right\rangle = \langle \langle \text{Tr}_b \tilde{\rho}_d \rangle \rangle \quad (9)$$

where now  $\tilde{\rho}_d$  is a solution of the stochastic equation

$$\frac{d\tilde{\rho}_d}{dt} = [v_j(t) Q_j + y_n(t) D_n + \mathcal{L} (H_d + x_n(t) D_n)] \tilde{\rho}_d \quad (10)$$

with the same random sources  $x_n(t)$  and  $y_n(t)$  (closely repeated indices imply summation).

Notice that (9) and (10) again exploit the Feynman-Kac type relations, now for stochastic evolution operator  $[y_n(t) D_n + \mathcal{L} (H_d + x_n(t) D_n)]$  in place of  $L$ , and that next such instants will not commented.

It is easy to see that  $x_n(t)$  surrogate Hamiltonian perturbation,  $H_d \rightarrow H_d + x_n(t) D_n$ , of “D” by “B”. What is for  $y_n(t)$ , they enter (8) and (10) like test functions conjugated with variables  $D_n$ . Therefore one can say that  $y_n(t)$  describe observation of “D” by “B”. But any thing under observation affects the observer. Hence, in other words,  $y_n(t)$  represent an opposite action of “D” onto “B”. Importantly, this passes without self-action of “D”, which is the reason for peculiarity of random processes  $y_n(t)$ : they are null by themselves ( $\langle \langle y_{n_1}(t_1) \dots y_{n_k}(t_k) \rangle \rangle = 0$ ) although possess non-zero cross-correlations with  $x_n(t)$  [4, 5, 6, 7, 8, 9]. Such correlations are responsible for energy dissipation in “D” and similar statistical effects.

Quantitatively, full statistics of  $x_n(t)$  and  $y_n(t)$  is determined by separate evolution of “B” under perturbations of its Hamiltonian,  $H_b \rightarrow H_b + f_n(t) B_n$ , by arbitrary time-varying forces  $f_n(t)$  [4, 5, 6, 7, 8]. In this section, let  $\Gamma \equiv \Gamma_b$ , and  $B_n(t', f, \Gamma)$  be values of the phase functions  $B_n$  considered at time  $t'$  as functionals of the forces and functions of current “B”’s state

$\Gamma = \Gamma(t)$  at time  $t$ . Then characteristic functional of  $x_n(t)$  and  $y_n(t)$  is

$$\begin{aligned} \Xi\{u(\tau), f(\tau)\} &\equiv \\ &\equiv \langle \langle \exp \int_{t>t'} [u_n(t') x_n(t') + f_n(t') y_n(t')] dt' \rangle \rangle = \\ &= \text{Tr}_b \rho_b(t, f, \Gamma) \exp \left\{ \int_{t>t'} u_n(t') B_n(t', f, \Gamma) dt' \right\} \quad (11) \end{aligned}$$

with  $\rho_b(t, f, \Gamma)$  being current “B”’s distribution function. Since  $B_n(t' = t, f, \Gamma) \equiv B_n(\Gamma)$ , the expression under the trace in (11),

$$\tilde{\rho}_b \equiv \rho_b(t, f, \Gamma) \exp \left\{ \int_{t>t'} u_n(t') B_n(t', f, \Gamma) dt' \right\} \quad ,$$

satisfies the differential equation

$$d\tilde{\rho}_b/dt = [u_n(t) B_n + \mathcal{L} (H_b + f_n(t) B_n)] \tilde{\rho}_b \quad , \quad (12)$$

quite similar to (10), and CF (11) can be evaluated by solving this equation:

$$\Xi\{u(\tau), f(\tau)\} = \text{Tr}_b \tilde{\rho}_b \quad (13)$$

Variational differentiations of (11) produce the identities

$$\left\langle \left\langle \prod_j x(t_j) \prod_m y(\tau_m) \right\rangle \right\rangle = \quad (14)$$

$$= \left[ \prod_m \frac{\delta}{\delta f(\tau_m)} \text{Tr}_b \rho_b(t, f, \Gamma) \prod_j B(t_j, f, \Gamma) \right]_{f=0}$$

clearly explaining the peculiarity of  $y_n(t)$ . Besides, (14) shows the nullity of any cross-correlations between  $y_n(\tau)$  and earlier  $x_n(t' \leq \tau)$  [4, 5, 6, 7, 8, 9], which is consequence of the causality principle (none perturbation of “D” by “B” can depend on future perturbations of “B” by “D”).

**IV. Fluctuation-dissipation relations.** The phase volume conservation and generic time-reversal and time-translation symmetries of Hamiltonian mechanics result in the Onsager reciprocity relations, Kubo formulas, fluctuation-dissipation theorems [1] and other “fluctuation-dissipation relations” (FDR) [12, 13, 14, 15].

In [8, 9] general quantum FDR were reconsidered in terms of the stochastic representation. To exploit their classical limit, let us assume, without loss of generality, that (i)  $f_n(-\infty) = f_n(+\infty) = 0$ , (ii)  $B_n$  are chosen so that their unperturbed mean values are zeroes (i.e.  $\langle \langle x_n(t) \rangle \rangle = 0$ ), and (iii)  $B_n$  possess definite time-reversal parities:  $B_n(q, -p) = \epsilon_n B_n(q, p)$  with  $\epsilon_n = \pm 1$ . Besides, assume, with a loss of generality, that (iv) the past initial distribution function of “B” (before switching-on the “D”-“B” interaction) was the canonical one,  $\propto \exp(-H_b/T)$ , and (v)  $H_b$  is even:

$H_b(q, -p) = H_b(q, p)$ . Then the classical generating FDR [12, 13, 14] yield

$$\Xi \left\{ u(\tau) - \frac{1}{T} \frac{df(\tau)}{d\tau}, f(\tau) \right\} = \Xi \{ \epsilon u(-\tau), \epsilon f(-\tau) \} \quad (15)$$

The same can be expressed [8] by the equalities

$$\begin{aligned} \epsilon_n x_n(-\tau) &\asymp x_n(\tau) , \\ \epsilon_n y_n(-\tau) &\asymp y_n(\tau) + T^{-1} dx_n(\tau)/d\tau , \end{aligned} \quad (16)$$

where symbol  $\asymp$  means statistical equivalence.

For example, averaging the product of two lines of (16) taken with different arguments, it is easy to obtain such second-order relation:

$$K_{jm}^{xy}(\tau) = \frac{\theta(\tau)}{T} \frac{d}{d\tau} K_{jm}^{xx}(\tau) , \quad (17)$$

where  $\theta(\tau)$  is the Heavyside step function,

$$K_{jm}^{xx}(\tau) \equiv \langle \langle x_j(\tau) x_m(0) \rangle \rangle , \quad K_{jm}^{xy}(\tau) \equiv \langle \langle x_j(\tau) y_m(0) \rangle \rangle ,$$

and the causality principle is accounted for as prescribed by (14).

**V. Distribution function.** Come back to “D” as described by the Eqs.7,8,9 and 10, using  $\Gamma \equiv \Gamma_d \equiv \{q, p\}$  as notation for complete set of “D”’s variables.

Equation (8) can be viewed as generating equation for CF of variables  $D_n$  in the system with Hamiltonian  $H_d + x_n(t)D_n$ . At that, as we already mentioned,  $y_n(t)$  play the role of test functions conjugated with  $D_n$ , while  $x_n(t)$  are external forces. This picture is described by Hamilton equations and Liouville equation as follow:

$$d\Gamma(t)/dt = -[\mathcal{L}(H_d + x_n(t)D_n)\Gamma](t) , \quad (18)$$

$$d\check{\rho}/dt = \mathcal{L}(H_d + x_n(t)D_n)\check{\rho} \quad (19)$$

Below, let  $\Gamma(t) = \Gamma(t, x, \Gamma, \theta)$  denote solution of Eq.18 with initial condition  $\Gamma(t = \theta) = \Gamma$ . Besides, define  $\check{\rho}(t, x, \Gamma)$  be solution of Eq.19 under condition  $\check{\rho}(t_0, x, \Gamma) = \rho_{d0}(\Gamma)$ , where  $\rho_{d0}$  is  $\Gamma$ ’s distribution at past initial time moment,  $t_0$ . Formally,  $t_0$  is the time when the “D”-“B” interaction was switched-on. Direct solution of (19) reads

$$\begin{aligned} \check{\rho}(t, x, \Gamma) &= \int \delta\{\Gamma - \Gamma(t, x, \Gamma_0, t_0)\} \rho_{d0}(\Gamma_0) d\Gamma_0 = \\ &= \int \delta\{\Gamma_0 - \Gamma(t_0, x, \Gamma, t)\} \rho_{d0}(\Gamma_0) d\Gamma_0 = \\ &= \rho_{d0}(\Gamma(t_0, x, \Gamma, t)) , \end{aligned} \quad (20)$$

where  $\delta\{\dots\}$  means delta-function in the phase space and  $\Gamma_0$  the initial state. At that, the group property of  $\Gamma$ ’s transformations from one time point to another:

$$\Gamma(t', x, \Gamma(t, x, \Gamma_0, t_0), t) = \Gamma(t', x, \Gamma_0, t_0) , \quad (21)$$

and the Liouville theorem about phase volume conservation were taken into account.

In these designations, solution of Eq.8 looks as

$$\tilde{\rho}_d = \check{\rho}(t, x, \Gamma) \exp \left\{ \int_{t_0}^t y_n(t') D_n(t', x, \Gamma, t) dt' \right\} \quad (22)$$

with  $D_n(t', x, \Gamma, t) \equiv D_n(\Gamma(t', x, \Gamma, t))$ .

Since  $y_n(t)$  are null by themselves and null in conjunction with any earlier  $x_n(t' \leq t)$ , while  $\check{\rho}(t, x, \Gamma)$  depends on  $x_n(t' < t)$  only, and  $\Gamma(t', x, \Gamma, t)$  depend on  $x_n(\min(t, t') < t'' < \max(t, t'))$  only, one can replace the upper integration limit in (22) by any value  $> t$ , in particular, by  $\infty$ . Then the exponent in (22) transforms into the statistically equivalent functional

$$S_t\{x, y, \Gamma\} \equiv \exp \left[ \int y_n(t') D_n(\Gamma(t', x, \Gamma, t)) dt' \right] \quad (23)$$

After this replacement, substitution of (22) to (7), with use of identities (20) and (21), yields

$$\rho_d(t, \Gamma) = \langle \langle \check{\rho}(t, x, \Gamma) S_t\{x, y, \Gamma\} \rangle \rangle = \quad (24)$$

$$= \int \langle \langle \delta\{\Gamma - \Gamma(t, x, \Gamma_0, t_0)\} S_{t_0}\{x, y, \Gamma_0\} \rangle \rangle \rho_{d0}(\Gamma_0) d\Gamma_0$$

Alternatively, by averaging directly formal operator solution of Eq.8, one obtains

$$\rho_d = \hat{\Theta} \exp \left\{ \int_{t_0}^t \mathcal{L}(H_d) dt' \right\} \Xi\{\mathcal{L}(D), D\} \rho_{d0} , \quad (25)$$

where  $\hat{\Theta}$  symbolizes chronological ordering of the following operator expression (that is ordering with respect to imaginary time argument of  $H_d$  and  $D_n$ ).

**VI. Fluctuation statistics.** Similarly to preceding section, consider Eq.10 as generating equation for joint CF of variables  $Q_j$  and  $D_n$ .

Now, express solutions of (18) and (19) through “D”’s state at arbitrary fixed time moment  $\theta$  which is different from  $t$ , that is solve (18) and (19) under initial condition  $\Gamma(t' = \theta) = \Gamma$  (thus  $\Gamma(t' = \theta, x, \Gamma, \theta) = \Gamma$ ). Then solution of Eq.10 can be implicitly formulated as

$$\begin{aligned} \tilde{\rho}_d(t, \Gamma(t, x, \Gamma, \theta)) &= \check{\rho}(\theta, x, \Gamma) \times \\ \exp \left\{ \int_{t > t'} [v_j(t') Q_j(t', x, \Gamma, \theta) + y_n(t') D_n(t', x, \Gamma, \theta)] dt' \right\} \end{aligned} \quad (26)$$

with  $Q_j(t', x, \Gamma, \theta) \equiv Q_j(\Gamma(t', x, \Gamma, \theta))$ . Substituting (26) to (9) and taking into account the Liouville theorem (the phase volume conservation under arbitrary Hamiltonian evolution), at  $t \rightarrow \infty$  we have

$$\langle \exp \left\{ \int v_j(t') Q_j(t') dt' \right\} \rangle = \langle \langle \text{Tr}_d \exp \left\{ \int v_j(t') Q_j(t', x, \Gamma, \theta) dt' \right\} \check{\rho}(\theta, x, \Gamma) S_\theta\{x, y, \Gamma\} \rangle \rangle \quad (27)$$

In terms of various statistical moments of variables  $Q_j$  (omitting their indices)

$$\langle Q(t_1) \dots Q(t_k) \rangle = \text{Tr}_d \langle \langle Q(t_1, x, \Gamma, \theta) \dots Q(t_k, x, \Gamma, \theta) \check{\rho}(\theta, x, \Gamma) S_\theta \{x, y, \Gamma\} \rangle \rangle \quad (28)$$

In particular, if  $\theta \rightarrow t_0$  then  $\check{\rho}(\theta, x, \Gamma)$  turns into the initial distribution,  $\rho_{d0}(\Gamma)$ , definitively independent on  $x_n(t)$ :

$$\langle Q(t_1) \dots Q(t_k) \rangle = \text{Tr}_d \rho_{d0}(\Gamma) \langle \langle Q(t_1, x, \Gamma, t_0) \dots Q(t_k, x, \Gamma, t_0) S_{t_0} \{x, y, \Gamma\} \rangle \rangle \quad (29)$$

with  $\Gamma$  representing the initial state  $\Gamma_0$ . The same expression results from (28) after substitution of (20) and (21).

Alternatively, quite similarly to (25),

$$\langle \exp \{ \int v_j(t') Q_j(t') dt' \} \rangle = \text{Tr}_d \hat{\Theta} \exp \{ \int [v_j(t') Q_j + \mathcal{L}(H_d)] dt' \} \Xi \{ \mathcal{L}(D), D \} \rho_{d0} \quad (30)$$

The functional  $\Xi$  here, defined by (11), at once accumulates all information about “B” which must be used when evaluating (27)-(29).

**VII. Self-interaction through environment and “scattering operator”.** It is useful to emphasize rather interesting resemblance between Eq.28 or Eq.29 and expressions for scattering amplitudes, Green functions, etc., in quantum theory of fields and many-particle systems (see e.g. [16, 17]). If draw an analogy from  $Q_j$  and  $x_n(t)$  to electron operators and radiation field, respectively, then the averages  $\langle \langle Q(t_1, x, \Gamma, t_0) \dots Q(t_k, x, \Gamma, t_0) \rangle \rangle$  correspond to lowest-order perturbation approximation, while  $\langle \langle Q(t_1, x, \Gamma, t_0) \dots Q(t_k, x, \Gamma, t_0) S_{t_0} \{x, y, \Gamma\} \rangle \rangle$  in Eq.29 exactly summarizes all the orders of “D”’s interaction with its environment. The analogy continues in that the “complete multiple scattering operator”  $S_{t_0} \{x, y, \Gamma\}$  by itself behaves like unity:

$$\langle \langle S_{t_0} \{x, y, \Gamma\} \rangle \rangle = 1 \quad (31)$$

This identity clearly follows from Eq.24 at  $t \rightarrow t_0$  and is easy explainable if notice that in any term of  $S_{t_0} \{x, y, \Gamma\}$ ’s series expansion over  $y_n(t')$  and  $x_n(t')$  most late time argument belongs to some of  $y$ ’s.

According to (11) and (14), separately  $x_n(t)$  are nothing but noise of free unperturbed environment, like “zero, or vacuum, fluctuations”. However, along with  $y_n(t)$  in

$S_{t_0} \{x, y, \Gamma\}$  they represent actual noise of the environment, including its directional response to the system’s motion, in the form of both renormalization of primordial “D”’s dynamical properties and appearance of new ones: relaxation, “spectral lines broadening”, etc.

**VIII. State-dependent noise and the fiction of friction.** In [4, 5, 6] the words “Langevin equation” were addressed to objects like (8) or (10) which emerged as stochastic extensions of the Liouville equation for probability measure of  $\Gamma$ . In usual sense, Langevin equations must be a stochastic extension of the Hamilton equations for  $\Gamma$  themselves. Besides, one would want these equations to involve some “realistic” noises only but not auxiliary “ghost” noises like  $y_n(t)$ . The latter requirement means that desirable equations are certainly not literal consequence of the basic Eqs.8 and 10. Instead, Langevin equations must be especially constructed as their exact statistical equivalent (or at least close approximate one).

It should be underlined that, at such target setting, a “size” of system “B” is insignificant (no matter e.g. is a Brownian particle macroscopic or as small as molecules).

With the formulated purpose, let us return to Eq.29, choosing arbitrary functions  $Q_j(\Gamma)$  as delta-functions  $\delta\{\Gamma - \gamma\}$  and their index as time. Then Eq.29 produces

$$W\{\gamma\} \equiv \langle \prod_t \delta\{\Gamma(t) - \gamma(t)\} \rangle = \int \langle \langle \prod_t \delta\{\Gamma(t, x, \Gamma_0, t_0) - \gamma(t)\} \exp \{ \int y(t) D(\gamma(t)) dt \} \rangle \rangle \rho_{d0}(\Gamma_0) d\Gamma_0 \quad (32)$$

which represents probability density functional for the whole system’s trajectory. Here all non-principal indices are omitted, and the delta-functions have allowed to replace  $D(\Gamma(t, x, \Gamma_0, t_0))$  in the exponent by  $D(\gamma(t))$ .

The simplest construction of Langevin equations follows directly from careful “visual” investigation of Eq.32. This shows that Eq.32 can be rewritten as

$$W\{\gamma\} = \int \langle \langle \prod_t \delta\{\Gamma(t, z, \Gamma_0, t_0) - \gamma(t)\} \rangle \rangle^\gamma \rho_{d0}(\Gamma_0) d\Gamma_0, \quad (33)$$

with new random forces  $z_n(t)$  in place of  $x_n(t)$ , if conditional statistics of  $z_n(t)$  is defined by formulas

$$\langle \langle z(t_1) \dots z(t_k) \rangle \rangle^\gamma \equiv \langle \langle x(t_1) \dots x(t_k) \exp \{ \int y(t) D(\gamma(t)) dt \} \rangle \rangle \quad (34)$$

The brackets  $\langle\langle \dots \rangle\rangle^\gamma$  here have the sense of conditional averaging under given system's trajectory  $\gamma(t)$ .

At that, the role of Langevin equations governing the variables  $\Gamma(t) \equiv \Gamma(t, z, \Gamma, t_0)$  and  $Q(t) \equiv Q(\Gamma(t, z, \Gamma, t_0))$  belongs to nothing but merely the Hamilton equations:

$$d\Gamma(t)/dt = -[\mathcal{L}(H_d + z_n(t)D_n)\Gamma](t) \quad (35)$$

Notice that in view of identity (31) the averaging procedure defined in (34) automatically satisfies the normalization condition  $\langle\langle 1 \rangle\rangle^\gamma = 1$ . Besides, due to the above mentioned statistical peculiarities of  $y(t)$ 's, result of the averaging always agrees with the causality principle: the moments (34) in fact can depend on  $\gamma(t)$  with  $t < \max(t_1, \dots, t_k)$  only.

Formally, the two above expressions, (34) and (35), already define what can be named "exactly equivalent Langevinian form of the stochastic representation". It clearly emphasizes statistical nature of dissipation and friction: even if being present they still are hidden inside  $z(t)$ 's statistics, as cross-correlations of  $x(t)$ 's with  $y(t)$ 's. To see them evidently in (35), we have to withdraw them from (34) in some reasonable approximation,

with corresponding redefinition of noises  $z_n(t)$ .

### IX. Unbiased noise and Langevin equations.

With the above pointed purpose, first, assume, naturally and without loss of generality, that  $\langle x \rangle = 0$ . Then desired dissipative contributions to (35), together with the renormalization corrections of non-dissipative terms, can be identified among mean values of  $z(t)$ 's.

Second, consider cumulants (semi-invariants)  $\kappa_{\alpha\beta} \equiv \langle\langle x_1, \dots, x_\alpha, y_1, \dots, y_\beta \rangle\rangle$ . For brevity, here the subscripts unify indices and time, and commas do emphasize that comma-separated multipliers are subject to purely irreducible correlation of  $(\alpha + \beta)$ -th order ("Malakhov's cumulant brackets"). Then CF (11) can be symbolically written as

$$\Xi\{u, f\} = \exp[\kappa\{u, f\}] \equiv \exp \left[ \sum_{\alpha=2}^{\infty} \kappa_{\alpha 0} \frac{u^\alpha}{\alpha!} + \sum_{\alpha, \beta=1}^{\infty} \kappa_{\alpha\beta} \frac{u^\alpha f^\beta}{\alpha! \beta!} \right]$$

(according to our assumption,  $\kappa_{10} = \langle x \rangle = 0$ ). Decompose it into two multipliers:

$$\Xi\{u, f\} = \Xi\{u, f\} \tilde{\Xi}\{u, f\}, \quad \Xi\{u, f\} \equiv \exp \left[ \sum_{\beta=1}^{\infty} \kappa_{1\beta} \frac{u f^\beta}{\beta!} \right], \quad \tilde{\Xi}\{u, f\} \equiv \exp \left[ \sum_{\alpha=2}^{\infty} \sum_{\beta=0}^{\infty} \kappa_{\alpha\beta} \frac{u^\alpha f^\beta}{\alpha! \beta!} \right] \quad (36)$$

Correspondingly to this factorization of CF, both the original noises,  $x(t)$ 's and  $y(t)$ 's, divides into two components:  $x = \bar{x} + \tilde{x}$  and  $y = \bar{y} + \tilde{y}$ , where two pairs  $\{\tilde{x}, \tilde{y}\}$  and  $\{\bar{x}, \bar{y}\}$  are mutually statistically independent.

It is easy to prove that for arbitrary functional  $\Phi(\bar{x})$  and arbitrary function  $f$  the equality holds as follows:

$$\langle\langle \Phi(\bar{x}) \exp(f\bar{y}) \rangle\rangle = \Phi(\bar{X}(f)), \quad \bar{X}(f) \equiv \sum_{\beta=1}^{\infty} \kappa_{1\beta} f^\beta / \beta! \quad (37)$$

This is because the pair  $\{\bar{x}, \bar{y}\}$ , in accordance with (14), describes merely conditional mean value of "B"'s response to its perturbation by forces  $f$ . Applying the decomposition (36) to (32), with the help of (37) we obtain

$$W\{\gamma\} = \int \langle\langle \prod_t \delta\{\Gamma(t, \bar{X}(D(\gamma)) + \tilde{x}, \Gamma_0, t_0) - \gamma(t)\} \exp\left\{ \int \tilde{y}(t) D(\gamma(t)) dt \right\} \rangle\rangle \rho_{d0}(\Gamma_0) d\Gamma_0 \quad (38)$$

The mean response  $\bar{X}(f)$ , defined by (37), with  $f = D(\gamma)$ , after restoration of its temporal index, reads

$$\bar{X}(t, f) = \frac{\delta}{\delta u(t)} \ln \Xi\{u, f\} |_{u=0} = \int \langle\langle x(t), y(t_1) \rangle\rangle f(t_1) dt_1 + \frac{1}{2} \int \int \langle\langle x(t), y(t_1), y(t_2) \rangle\rangle f(t_1) f(t_2) dt_1 dt_2 + \dots, \quad (39)$$

where because of (14) all integrals are in fact taken over  $t_j < t$ . It is useful to notice also that, due to the causality, Jacobian of mutual transformations between  $\gamma$  and  $\Gamma$  is unit.

Scanning (38) in comparison with (32) and (33), one evidently comes to another form of the probability functional:

$$W\{\gamma\} = \int \langle \langle \prod_t \delta\{\Gamma(t, \bar{X}(D(\gamma)) + \tilde{z}, \Gamma_0, t_0) - \gamma(t)\} \rangle \rangle^\gamma \rho_{d0}(\Gamma_0) d\Gamma_0 , \quad (40)$$

where statistics of renormalized (in fact merely biased) noises  $\tilde{z}(t)$  is now described by

$$\langle \langle \tilde{z}(t_1) \dots \tilde{z}(t_k) \rangle \rangle^\gamma \equiv \langle \langle \tilde{x}(t_1) \dots \tilde{x}(t_k) \exp \left\{ \int \tilde{y}(t) D(\gamma(t)) dt \right\} \rangle \rangle \quad (41)$$

At that, correspondingly to (40),  $\Gamma(t) = \Gamma(t, \bar{X}(D(\Gamma)) + \tilde{z}, \Gamma_0, t_0)$ , that is stochastic Hamilton equations (35) change to the stochastic integro-differential equations

$$d\Gamma(t)/dt = -[\mathcal{L}(H_d)\Gamma](t) - (\bar{X}_n(t, D(\Gamma)) + \tilde{z}_n(t)) [\mathcal{L}(D_n)\Gamma](t) \quad (42)$$

As prescribed by (36) and (41), here the noises  $\tilde{z}_n(t)$  have certainly zero mean values, while any dissipative effects of interaction with “B” are separated in  $\bar{X}_n(t, D(\Gamma))$ . Hence, Eqs.42 can be by now enough surely named “Langevin equations”.

**X. Discussion.** Of course, the above result is rather trivial one. However, from the point of view of applications and practical computability, it is not quite satisfactory. The matter is that numeric modeling of noise essentially conditioned by the system it drives is generally difficult task. It would be better if the noise was reduced to unconditioned random quantities, for example,

$$\tilde{z}(t) = z^{(0)}(t) + \int z^{(1)}(t, t_1) f(t_1) dt_1 + \frac{1}{2} \int \int z^{(2)}(t, t_1, t_2) f(t_1) f(t_2) dt_1 dt_2 + \dots , \quad (43)$$

where  $z^{(0)}(t) = \tilde{x}(t) = x(t)$  is unperturbed noise,  $z^{(1)}(t, t_1)$  represents stochastic linear response of “B” to its perturbation, etc., and all  $z^{(n)}$  are some zero-average random functions independent on the forces. In particular,  $z^{(1)}(t, t_1)$  includes fluctuations in linear friction (whose average was contained in first term of (39)).

The only situation when Eqs.42 finalize the analysis is when the noises  $\tilde{z}(t)$  are state-independent, that is  $z^{(n)} = 0$  for all  $n > 0$ . But this is unlikely realistic situation since in general it is forbidden by restrictions which follow from the phase volume conservation and microscopic reversibility. For concreteness, if “B” is equilibrium thermal bath (thermostat), these restrictions are expressed by FDR (15) [12, 13, 14, 15] or equivalently (16) (notice that FDR for internally non-equilibrium baths also were considered in [12, 13]). If noises  $\tilde{z}(t)$  are indeed state-independent, this means that  $\kappa_{\alpha\beta} = 0$  for all  $\alpha \geq 2$  and  $\beta \geq 1$ . Then the second row from (16) clearly implies that in such case the equalities  $\kappa_{\alpha 0} = 0$  also should hold for all  $\alpha \geq 3$ . In other words, the noise  $\tilde{z}(t)$  can be purely state-independent only when it is purely Gaussian. Moreover, then the same FDR prescribe that  $\kappa_{1\beta} = 0$  for all  $\beta \geq 2$ , that is average response of “B” is purely linear.

Thus we come to the trite “linear Gaussian thermo-

stat” when Eqs.41 and 39 reduce to

$$\bar{X}_n(t, D(\Gamma)) = -K_{nm}^{xx}(0) D_m(\Gamma(t))/T + \quad (44)$$

$$+ \frac{1}{T} \int_{-\infty}^t K_{nm}^{xx}(t-t') \frac{d}{dt'} D_m(\Gamma(t')) dt' ,$$

$$\langle \langle \tilde{z}_n(t_1) \tilde{z}_m(t_2) \rangle \rangle^\gamma = K_{nm}^{xx}(t_1 - t_2)$$

Here FDR (17) is used, and it is taken in mind that all higher-order cumulants of  $\tilde{z}(t)$  are zeros. Discussion of more interest models will be done elsewhere.

**XI. Example: oscillator.** Consider nonlinear oscillator, assuming that “B” is “linear Gaussian thermostat” while interaction with it realizes in potential way through two statistically independent channels as follow:

$$H_d = p^2/2m + U_0(q) , \quad D_1(\Gamma) = -q , \\ D_2(\Gamma) = q^2/2 , \quad K_{12}^{xx} = K_{21}^{xx} = 0$$

The first channel corresponds to usual thermal excitation, and the second to thermal parametric fluctuations in frequency of oscillations. The Eqs.42 and 44 yield

$$dq(t)/dt = p(t)/m ,$$

$$dp(t)/dt = -dU(q(t))/dq(t) + \tilde{x}_1(t) + \tilde{x}_2(t) q(t) - \\ - \int_{-\infty}^t K_{11}^{xx}(t-t') v(t') dt' / T - \\ - q(t) \int_{-\infty}^t K_{22}^{xx}(t-t') q(t') v(t') dt' / T , \quad (45)$$

where  $v(t) \equiv dq(t)/dt$  is velocity,  $\tilde{x}_n(t)$  are mutually independent normal random processes,  $K_{nn}^{xx}$  are their correlators, and

$$U(q) \equiv U_0(q) - K_{11}^{xx}(0) q^2/2T - K_{22}^{xx}(0) q^4/8T$$

is renormalized potential. Hence, correspondingly, there are two channels of friction and dissipation, and the friction channel conjugated with thermal parametric fluctuations is essentially nonlinear. Similar examples concerning thermal fluctuations in capacities of electric circuits were considered in [18].

**XII. Conclusion.** For particular variant of the “stochastic representation of deterministic interactions” concerning classical Hamiltonian mechanics, we have demonstrated that by request it can be completely reformulated in terms of “Langevin equations” for internal variables of an open system. These equations are wholly housed in its own phase space and are free of the peculiar auxiliary noises  $y_n(t)$ , distinctive for initial “stochastic representation”. At the same time,  $y_n(t)$  remain useful undercover instrument, being responsible for conditional statistical dependence of actual noise on trajectory of the system driven by it.

This Langevinian form of the theory seems more vivid, although, probably, it will occur less appropriate for practical analysis of complicated noise statistics. Besides, the

original “Liouvillian form” at once covers quantum mechanics as well.

What is for its quantum Langevinian equivalent, still it remains unexplored. Notice that quantum Langevin equations for important special case of Gaussian linear thermostat were exhaustively considered in [19]. Of course, more general situations also were under many considerations (see e.g. [20]).

But recall that the question under our principal and pragmatic interest is how much non-Gaussian non-linear generalization of quantum Langevin equations can be developed if do it wholly within native Hilbert space of an open system under consideration and with use of commutative ( $c$ -number valued) noise sources only.

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